I. General Information

CAS Number: C.I. Pigment Red 49 (Barium) (CAS NO.:1103-38-4)

Name: 1-Naphthalenesulfonic acid, 2[(2-hydroxy-1-(Naphthalenyl)azo]-,barium

II. Physical-Chemical Data

A1. Melting Point

Test Substance

Test substance: Benzenesulfonic acid, 5 chloro-2-[(2-hydroxy-1-naphthalenyl) azo]-4-methyl-barium salt (R53)

Remarks:

Method

Method: Measured

Remarks:

Results

Melting point value:

Remarks: 330 °C

References

Unpublished company data reliable with restrictions. Hoechst AG (1992) Unveroeffenlichte Untersuchung Der Abt. Analytisches Laboratorium (17.11.1992)

Other

Data is consistent with melting points for the class of pigments and other available measurements

A2. Melting Point

Test Substance

Test substance: 1-Naphthalenesulfonic acid, 2[(2-hydroxy-1-(Naphthalenyl) azo]-,barium R 49)

Remarks:

Method

Method: Estimation

Remarks:

Results

Melting point value: 349.84 °C

Remarks:

References

MPBPWIN v1.40 in EPIWIN v 3.10, Syracuse Research Corporation, Syracuse, New York

Other

Data is consistent with melting points for the class of pigments and other available measurements.

B. **Boiling Point**

Test Substance

Test substance: SOLID N/A

Remarks:

Method

Method:

Remarks:

Results

Boiling point value:

Remarks:

References

Other

C1. **Vapor Pressure**

Test Substance

Test substance: 1-Naphthalenesulfonic acid, 2[(2-hydroxy-1-(Naphthalenyl)azo]-,barium R 49)

Remarks:

Method

Method: Estimation

Remarks: Modified Grain method

Results

Vapor pressure value: 4.62 E-015 mm Hg

Temperature:

Remarks:

References

MPBPWIN v1.40 in EPIWIN v3.10, Syracuse Research Corporation, Syracuse, New York

Other

D. Partition Coefficient

Test Substance

Test substance:	Benzenesulfonic acid, 5 chloro-2-[(2-hydroxy-1-naphthalenyl)azo]-4-methyl-barium salt R 53)
Remarks:	

Method

Method:	Estimated
Remarks:	

Results

Log P_{OW}:	-.56
Remarks:	

References Hoechst AG (1997) : Unveroeffentlichte Untersuchung Pigmentanalytik (25.02.1997) SIDS Dossier C.I. Pigment Red 53

Other

E. Water Solubility

Test Substance

Test substance:	Benzenesulfonic acid, 5 chloro-2-[(2-hydroxy-1-naphthalenyl)azo]-4-methyl-barium salt R 53)
Remarks:	

Method

Method:	
Remarks:	Estimated

Results

Value:	2 mg/L
Temperature:	25 °C??
Description:	
Remarks:	Very Low Solubility

References

Hoechst AG (1993):Unveroeffentlichte Untersuchung (93.0358) SIDS Dossier, C.I. Pigment Red 53

Other

III. Environmental Fate Endpoints

A. Photodegradation

Test Substance

Test substance: 1-Naphthalenesulfonic acid, 2[(2-hydroxy-1-(Naphthalenyl)azo]-,barium R 49)

Remarks:

Method

Method: Estimate
Test type: Water\sunlight
Remarks:

Results

Temperature:
Degradation Rate
18.6 E-12
: Half-life
Ozone reaction: 6.9 Hours ?? **(or not readily degradable, estimation not possible??)**
Remarks:

Conclusions

References

AopWin v1.90 in EPIWIN v 3.10, Syracuse Research Corporation, Syracuse, New York

Other

A2. Photodegradation

Test substance: Benzenesulfonic acid, 5 chloro-2-[(2-hydroxy-1-naphthalenyl)azo]-4-methyl-barium salt R 53)

Remarks:

Method

Method: Estimation
Test type: Water
Remarks:

Results

Temperature:
Hydroxyl radicals reaction
OH Rate constant:
Half-life estimation not possible
Ozone reaction:
Remarks:

Conclusions

References

Hoechst AG (1991):Einstufungsbegrundung TA-Luft der Abt.UCV (19.07.1991) IUCLID dataset C.I. Pigment Red 53

Other

B. Stability in Water

Test Substance

Test substance:	1-Naphthalenesulfonic acid, 2[(2-hydroxy-1-(Naphthalenyl)azo]-,barium R 49)
Remarks:	

Method

Method:	
Test type:	Estimation
GLP:	abiotic hydrolysis
Remarks:	Yes

Results

Half-life:	Hydrolysis rate cannot be estimated
Percent hydrolyzed in 5 days (120 hs) at 50 °C :	
Remarks:	

Conclusions

Data Quality

Remarks:

References EPIWIN v 3.10, Syracuse Research Corporation, Syracuse, New York

Other

C. Biodegradation

Test Substance

Test substance:	Benzenesulfonic acid, 5 chloro-2-[(2-hydroxy-1-naphthalenyl)azo]-4-methyl-barium salt R 53)
Remarks:	

Method

Method:	OECD 301C
Test type:	MITI 1 and Zahn Wellens Inherent biodegration
GLP:	Yes
Year:	(1992)
Remarks:	No biodegradation (MITI 1 Japanese standard activated sludge)

Results

Results:	33% eliminated after 21 days in Zahn Wellens test, 10 % of elimination due to adsorption onto the sludge
Remarks:	

Conclusions

Data Quality

Remarks:	This is a well-documented study.

References

Ministry of International Trade and Industry (MITI) (1992) Biodegradation and Bioaccumulation data for existing chemicals based on the Chemical Substances Control Law, Japan Chemicals Inspection and Testing Institute; Japan Chemical Industry Ecology - Toxicology and Information Center 14-19, 5-43, See also IUCLID dataset and SIDS DOSSIER C.I. Pigment Red 53.

Other

D. Transport between Environmental Compartments (Fugacity)

Test Substance

Test substance: 1-Naphthalenesulfonic acid, 2[(2-hydroxy-1-(Naphthalenyl)azo]-,barium
Remarks: R 49)

Method

Test type:
Model used: Estimation
Level III Fugacity Model; EPIWIN:EQC from Syracuse Research
Remarks: Corporation

Results

Model data and results:

	Distribution (%)
Air	.0791
Water	2.06
Soil	38.7
Sediment	59.2

Remarks: Since no experimental values were available the physical chemical values utilized in this model were default parameters from within EPIWIN.

Conclusions

References

Meylan, W. (1993). User's Guide for the Estimation Programs Interface (EPI), Version 3.10, Syracuse Research Corporation, Syracuse, New York 13210. The Level III model incorporated into EPIWIN is a Syracuse Research Corporation adaptation of the methodology described by Mackay *et al.* 1996; *Environ. Toxicol. Chem.* **15(9)**, 1618-1626 and 1627-1637.

Other

IV. Ecotoxicity

A. Acute Toxicity to Fish

Test Substance

Test substance:	Benzenesulfonic acid, 5 chloro-2-[(2-hydroxy-1-naphthalenyl)azo]-4-methyl-barium salt R 53)
Remarks:	

Method

Method:	Method 84/449/EEC
Test type:	Static system
GLP:	Yes
Year:	1982
Species/strain:	Brachydanio rerio
Analytical monitoring:	
Exposure period:	96-Hour
Remarks:	A group of 10 fishes were exposed to 5 nominal concentrations (17.1-180), DMSO Control(.5mg/l)and laboratory water control

Results

Nominal concentration:	
Measured concentration:	
Endpoint value:	96-hour LC_{50} >500mg/L
Biological observations:	
Statistical methods:	
Remarks:	

Conclusions

Data Quality

Reliability:	Reliable without restriction
Remarks:	

References

Hoechst AG (1982) :Unveroeffentlichte Untersuchung (82.0250). See also EUCLID Dataset C.I. Pigment Red 53 and SIDS Dossier C.I. Pigment Red 53

Other

A2. Acute Toxicity to Fish

Test Substance

Test substance:	Benzenesulfonic acid, 5 chloro-2-[(2-hydroxy-1-naphthalenyl)azo]-4-methyl-barium salt
Remarks:	

Method

Method:	
Test type:	Semistatic system
GLP:	Yes
Year:	1982
Species/strain:	Oryzias latipes (Orange Killifish)
Analytical monitoring:	
Exposure period:	48-Hour
Remarks:	

Results

Nominal concentration:	
Measured concentration:	48 hour LC_{50} >500 mg/L
Endpoint value:	
Biological observations:	
Statistical methods:	
Remarks:	

Conclusions

Data Quality

Reliability:	Reliable without restrictions
Remarks:	

References

Hoechst AG (1982) :Unveroeffentlichte Untersuchung (82.0250). See also EUCLID Dataset C.I. Pigment Red 53 and SIDS Dossier C.I. Pigment Red 53

Other

B. Acute Toxicity to Aquatic InvertebratesTest

Substance

Test substance:

Remarks: Benzenesulfonic acid, 5 chloro-2-[(2-hydroxy-1-naphthalenyl)azo]-4-methyl-barium salt R 53)

Method

Method:	OECD 202.
Test type:	Saturated solution
GLP:	Yes
Year:	1993
Species/strain:	Daphnid (*Daphnia magna*)
Analytical monitoring:	
Exposure period:	
Remarks:	

Results

Nominal concentration:	
Measured concentration:	
Endpoint value:	Saturated solution
Reproduction	48 -hour EC_{50} >2mg/l
Biological observations:	
Statistical methods:	
Remarks:	

Conclusions

Data Quality

Reliability: Reliable without restriction

Remarks: This was a well-documented OECD guideline study.

References

Hoechst AG (1993):Unveroeffentlichte Untersuchung (93.0358)
See also EUCLID dataset and SIDS Dossier, C.I. Pigment Red 53

Other

C. Toxicity to Aquatic Plants

Test Substance

Test substance:	1-Naphthalenesulfonic acid, 2[(2-hydroxy-1-(Naphthalenyl)azo]-,barium ® 49)
Remarks:	

Method

Method:	Estimation
Test type:	
GLP:	
Year:	
Species/strain:	
Endpoint basis:	
Exposure period:	
Analytical procedures:	
Remarks:	The conduction of an algae test with C.I. Pigment Red 49 is problematic as the substance leads to a strong coloring of the test solution and therefore to a reduction of light intensity. Therefore, the assessment is made on the basis of the above short term tests and computer model estimation.

Results

Nominal concentration:	
Measured concentration:	
Endpoint value:	
NOEC:	
Biological observations:	
Was control response satisfactory:	EC 50, 96 Hour .038 mg/L
Statistical Methods:	
Remarks:	

Conclusions

Data Quality

Reliability:	
Remarks:	

References reliable with restriction

Other

EPIWIN v 3.10, Syracuse Research Corporation, Syracuse, New York

V. Toxicological Data

A. Acute Toxicity

Test Substance

Test substance:	1-Naphthalenesulfonic acid, 2[(2-hydroxy-1-(Naphthalenyl)azo]-,barium ® 49)
Remarks:	Purity was unknown

Method

Method:	Acute lethality; Other
Test type:	LD_{50} estimate
GLP:	No (Pre-GLP)
Year:	1968
Species/strain:	Rat/unknown
Route of exposure:	Oral gavage
Dose levels:	Unknown
Remarks:	

Results

Value:	LD_{50} = >5,000 mg/kg.
Deaths at each dose:	
Remarks:	

Conclusions Material would be considered as not toxic.

Data Quality

Reliability:	Reliable with restrictions
Remarks:	The study was conducted quite some time ago and hence many study details are missing from the report and not available. However, basic data are given and results are consistent with other data for pigments of this class.

References Mone J.G. 1968, Federation Series on Coating Technology, Unit 9 Organic Pigments, Federation of Societies for Paint Technology, Philadelphia, PA 19107.

Other

Acute toxicity

Test substance:	Benzenesulfonic acid, 5 chloro-2-[(2-hydroxy-1-naphthalenyl)azo]-4-methyl-barium salt ® 53)
Remarks:	Purity was unknown

Method

Method:	Acute lethality; Other
Test type:	LD_{50} estimate
GLP:	No (Pre-GLP)
Year:	1977
Species/strain:	Rat and mouse
Route of exposure:	Oral gavage
Dose levels:	Unknown
Remarks:	

Results

Value:	LD_{50} = >10,000 mg/kg.
Deaths at each dose:	
Remarks:	

Conclusions Material would be considered as not toxic.

Data Quality

Reliability:	Reliable with restrictions
Remarks:	

References Hoechst AG (1977):Unveroffentl. Unters (Ber.-Nr. 77.0525. See also EUCLID Dataset and SIDS DOSSIER C.I. Pigment Red 53

Other

Acute Inhalation Toxicity LC50 > 4.13 mg/l, 1993, GLP study, Hoechst AG (1977):Unveroffentl. Unters (Ber.-Nr. 93.0427)

Repeated Dose Toxicity Test

Substance

Test substance:	Benzenesulfonic acid, 5 chloro-2-[(2-hydroxy-1-naphthalenyl)azo]-4-methyl-
Remarks:	barium salt (R53)

Method

Method:	
Test type:	Repeated subchronic dose
GLP:	Unknown
Year:	1982
Species/strain:	Rat Male and Female, Mice male and Female
Route of exposure:	Gavage
Duration of test:	91 days
Exposure levels:	Rats 0. 3000,6,000, 12,500, 25,000, or 50,000 ppm Mice 0,600,12,500,2,500,5,000, 10,000
Sex:	Male and Female Rats and Mice
Exposure period:	91 days
Post-exposure observation	
Remarks:	

Results

NOAEL (NOEL):

90 mg/kg mice, 25 mg/kg rats
After repeated oral administration for 90 days in rats pigment red 53:1 led in high dosages (at 3000 ppm and above) to hematological findings (depressed hemoglobin and hematocrit values) and effects on spleen (splenomegaly, haemosiderosis, fibrosis), liver and kidneys (heamosiderosis). Daily administration of pigment red 53:1 for 90 days in mice led to comparable findings. The NOEL for mice was determined as 90 mg/kg bw/day.

Conclusions Test substance is not significantly toxic

Data Quality

Reliability:	Reliable without restriction
Remarks:	

References: Carcinogenesis Bioassay of D & C Red No. 9 In F344 Rats and B6C3F1 Mice National Toxicology Program Technical Report Series No. 225. **See also EUCLID** dataset C.I. Pigment Red 53 for other studies conclusions consistent.

Other

C. Genetic Toxicity - Mutation

Test Substance

Test substances:	1-Naphthalenesulfonic acid, 2[(2-hydroxy-1-(Naphthalenyl)azo]-,barium **and** Benzenesulfonic acid, 5 chloro-2-[(2-hydroxy-1-naphthalenyl)azo]-4-methyl-barium salt ® 49 and R 53)
Remarks:	

Method

Method:	In Vitro Mutagenicity
Test type:	Ames
GLP:	Unknown
Year:	Unknown
Species/strain:	Salmonella typhimurium
Metabolic activation:	Yes, barium salt (and manganese salt)
Concentration tested:	
Remarks:	

Results

Result:	Negative
Cytotoxic concentration:	
Precipitation concentration:	
Genotoxic effects	
With activation:	Negative
Without activation:	Negative
Statistical methods:	
Remarks:	

Conclusions

Data Quality

Reliability:	Reliable with restrictions
Remarks:	

References

Brown, J.P., P.S. Dietrich & C. M. Bakner, 1979, "Mutagenicity testing of some drug and cosmetic dye lakes with salmonella/mammalian microsome assay," Mutat. Res., 66, 181-185., Muzzall, J.M. & W.L.Cook, 1979 "Mutagenicity test of dyes used in cosmetics with salmonella/ mammalian microsome test", Mutat. Res., 67,1-8 ,Milvy, P. & K. Kay 1978 "Mutagenicity of 19 major graphic arts and printing dyes, J. Toxcol. Environ. Health, 4, 31-6 NPIRI Raw Materials Handbook, 2000

C. Genetic Toxicity - Mutation

Test substance:	Benzenesulfonic acid, 5 chloro-2-[(2-hydroxy-1-naphthalenyl)azo]-4-methyl-barium salt
Remarks:	® 53)

Method

Method:	OECD 471
Test type:	Ames
GLP:	Yes
Year:	1985
Species/strain:	Salmonella typhimurium
Metabolic activation:	With and without
Concentration tested:	4 - 5000 ug/plate with and without activation
Remarks:	

Results

Result:	Negative in all bacterial strains with and without activation
Cytotoxic concentration:	
Precipitation concentration:	
Genotoxic effects	
With activation:	Negative
Without activation:	Negative
Statistical methods:	
Remarks:	

Conclusions

Data Quality

Reliability: Reliable without restriction Remarks:

References Hoechst AG (1977):Unveroffentl. Unters (Ber.-Nr. 85.0974). See also EUCLID dataset and SIDS DOSSIER C.I. Pigment Red 53

Other

D. Genetic Toxicity – Chromosomal Aberrations

Test Substance

Test substance:	Benzenesulfonic acid, 5 chloro-2-[(2-hydroxy-1-naphthalenyl)azo]-4-methyl-barium salt ® 53)
Remarks:	

Method

Method:	OECD 473
Test type:	Cytogenetics Assay
GLP:	Yes
Year:	1989
Species/strain:	Chinese Hamster CHL Cells
Exposure period:	
Remarks:	

Results

Result:	Negative
Genotoxic effects:	Negative
Concentration tested	30, 150,300 ug/ml
Statistical methods:	
Remarks:	

Conclusions Not mutagenic

Data Quality

Reliability:	Reliable without restriction
Remarks:	

References Hoechst AG (1977): Unveroffentl. Unters (Ber.-Nr. 89.1443). See also EUCLID dataset and SIDS DOSSIER C.I. Pigment Red 53

Other

E. **Developmental Toxicity**

Test Substance See 30 Month toxicity study below

Test substance:

Remarks:

Method

Method:

GLP:

Year:

Species/strain:

Sex:

Route of exposure:

Exposure levels:

Actual doses received:

Exposure period:

Duration of test:

Remarks:

Results

Maternal toxicity NOEL:

NOEL for teratogenicity:

NOEL for fetotoxicity:

Parental toxic responses:

Fetal toxic responses dose:

Statistical Methods:

Remarks:

Conclusions

Data Quality

Reliability:

Remarks:

References

Other

F. Toxicity to Reproduction

Test Substance

Test substance:	Benzenesulfonic acid, 5 chloro-2-[(2-hydroxy-1-naphthalenyl)azo]-4-methyl-barium salt
Remarks:	

Method

Method:	30 month Chronic Toxicity and Potential Carcinogenicity Study in Rats with In Utero and Lifetime Exposure to D & C Red No. 9 in the Diet
GLP:	no
Year:	1981
Species/strain:Sex:	Rat male and female
Route of exposure:	gavage
Exposure levels:	0, 10,000 mg/kg
Exposure period:	30 Months
Duration of test:	
Remarks:	

Results

Maternal toxicity NOEL:	NOEL< 10,000 ppm
Parental toxic responses:	NOEL >10,000 ppm
Fetal toxic responses dose:	NOEL >10,000 ppm (F1)
Statistical Methods:	
Remarks:	The purpose of a 30-months chronic toxicity and potential carcinogenicity study in rats with in utero and lifetime exposure to D & C Red No. 9 (pigment red 53:1) via its incorporation into the basal diets at doses of 0 and 10,000 ppm also was to evaluate the reproductive performance of the F0 generation. Rats of the Charles river CD strain were 35 days of age when treatment was initiated. After nine weeks of treatment, the animals were mated by pairing for seven days. The effect of test material for the in-utero phase was evaluated via mortality, clinical observations, body weight, food consumption, sex ratio, pup viability data and gross necropsy observations on selected animals. .

Conclusions There was no evidence for an impairment of reproductive functions in animals

Data Quality

Reliability:	
Remarks:	

References Reliable with restriction, this is a well documented study.

Other

Litton Bionetics Study for the Cosmetic, Toiletry and Fragrance Association, Inc. LBI Project Number 20832, June 1981,

Acute toxicity

Test substance: 1-Naphthalenesulfonic acid, 2[(2-hydroxy-1-(Naphthalenyl)azo]-,barium **and** Benzenesulfonic acid, 5 chloro-2-[(2-hydroxy-1-naphthalenyl)azo]-4-methyl-barium salt

Remarks:

Method

Method: Irritation to the rabbit eye
Test type: eye irritation
GLP: unknown
Year: ??
Species/strain: rabbit
Route of exposure:
Dose levels:
Remarks:

Results

Value: ??negative
Deaths at each dose:
Remarks:

Conclusions

Data Quality

Reliability: un-assignable
Remarks:

References **?? Company data [Need study or summary thereof]**

Other

Acute toxicity

Test substance:	1-Naphthalenesulfonic acid, 2[(2-hydroxy-1-(Naphthalenyl)azo]-,barium **and** Benzenesulfonic acid, 5 chloro-2-[(2-hydroxy-1-naphthalenyl)azo]-4-methyl-barium salt
Remarks:	

Method

Method:	Skin irritation to the rabbit
Test type:	Skin irritation
GLP:	unknown
Year:	
Species/strain:	rabbit
Route of exposure:	
Dose levels:	
Remarks:	

Results

Value:	negative
Deaths at each dose:	
Remarks:	

Conclusions

Data Quality

Reliability:	un-assignable
Remarks:	

References **Company data [need study or summary thereof]**

Other

Chronic Dose Toxicity Test Substance

Test substance: 1-Naphthalenesulfonic acid, 2[(2-hydroxy-1-(Naphthalenyl)azo]-,barium

Method

Method:	Chronic Toxicity
Test type:	Repeated oral dose
GLP:	unknown
Year:	1963
Species/strain:	Rat
Route of exposure:	Oral gavage
Duration of test:	two years
Exposure levels:	
Sex:	
Exposure period:	
Post-exposure observation period:	
Remarks:	

Results

NOAEL (NOEL):

No cancerous response. No toxicity or mortality as a result of exposure

Conclusions

Data Quality

Reliability: un-assignable

Remarks:

References

Davis, K.J. & O.G. Fitzhugh, 1963, "Pathologic changes noted in rats fed D & C Red No. 10 for two years", Toxicol. Appl. Pharmacol.,4, 200-205

Other